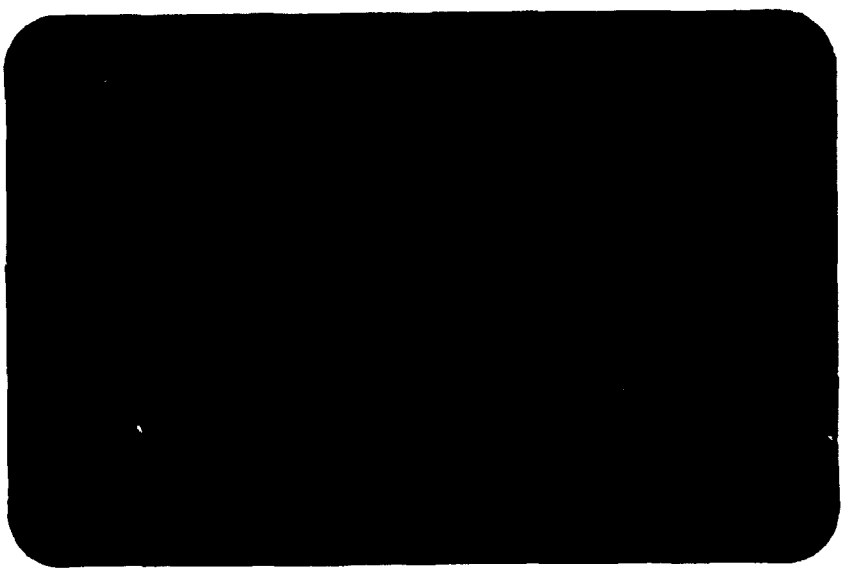
INSTITUTO DE FÍSICA

preprint



UNIVERSIDADE DE SÃO PAULO
INSTITUTO DE FÍSICA
Caixa Postal - 20.516
Cidade Universitária
São Paulo - BRASIL

IFUSP/P-121

ON THE NUMERICAL TREATMENT OF THE GRIFFIN-HILL-WHEELER EQUATION

D.Galetti[+] and A.F.R. de Toledo Piza

Instituto de Física, Universidade de São Paulo,
C.Postal 8219, São Paulo, S.P - Brasil

[+] Supported by Fundação de Amparo à Pesquisa do Estado de São Paulo.

ABSTRACT

The precision attainable in the numerical treatment of the Griffin-Hill-Wheeler equation is studied in a solvable model. Trucation errors related to the generator coordinate kinematics are exhibited and briefly discussed.

The generator coordinate method[1,2] has been extensively applied to the calculation of nuclear collective properties[3-5] although the limitations inherent to the numerical methods appear not to have been clearly exposed. In this note we discuss this problem in the context of a solvable model and using results of a previous work[6].

We will focus mostly on the procedure followed in ref.3. The problem is to obtain solutions for an equation of this type

$$\int \left[K(\alpha,\alpha') - E\, N(\alpha,\alpha') \right] f(\alpha')\, d\alpha' = 0 \qquad (1)$$

where

$$K(\alpha,\alpha') = \langle \alpha | H | \alpha' \rangle$$

and

$$N(\alpha,\alpha') = \langle \alpha | \alpha' \rangle$$

are the energy and overlap kernels respectively. To this end one evaluates the overlap kernel N for a set of (often equally spaced) mesh points on a given interval of the generator coordinate α. The resulting overlap matrix is diagonalized and one truncates the space of its eigenvectors by neglecting those associated with eigenvalues smaller than some small number ε. In the resulting subspace one defines

$$N^{\frac{1}{2}} f = g,$$

which can be used to rewrite (1) as

$$N^{-\frac{1}{2}} K N^{-\frac{1}{2}} g = Eg \qquad (2)$$

The diagonalization of the modified energy matrix $N^{-\frac{1}{2}} K N^{-\frac{1}{2}}$

gives them E and g. Usual checks on the numerical results are based on their stability with respect to a) changes in the number of mesh points for a given interval and truncation level ε ; b) change of the basic interval in a) for fixed ε; and c) change of ε.

In calculations performed along these lines, such as those of Flocard and Vautherin [3], these checks are considered in connection with the collective amplitudes g and with the eigenvalues E. It is in fact well known that the weights f associated with stable amplitudes g are themselves often unstable on the account of the non-orthogonal character of the representation is terms of the generator states[6,7]. As shown in refs.6 and 7, however this happens when the eigenvalues of the overlap kernel decrease faster than the probabilities of the corresponding eigenvectors for the state described by g. In such cases, the adoption of some definite truncation level ε for the eigenvalues of the overlap kernel may result in a dangerous truncation of the available phase-space. The actual quantitative importance of this truncation depends, however, on dynamical ingredients related to the nature of the energy kernel K. To some extent, it is revealed by lack of stability under the conditions given above, especially under condition c). Stability is however not a sufficient condition for convergence of the collective amplitude g, as the effect of some relevant states may be beclouded by the unavoidable numerical noise. Whether or not this happens will in each case depend on the adopted generator coordinate scheme in relation to the dynamical ingredients of the calculation.

The existence of truncation errors of this type can be demonstrated by comparing numerical results with the exact

solution of the collective hamiltonian [illegible] from a Griffin-Hill-Wheeler equation. A soluble problem which is suited for this purpose is the standard Gaussian Overlap Approximation in which the ratio K/N is expanded up to second order terms in $(\alpha - \alpha')$ and $(\alpha + \alpha')$ about a saddle point which represents a stable equilibrium situation for the collective degrees of freedom [2]. In fact, by varying the expansion coefficients at this saddle point we may sweep a range of different situations, including some for which the weight function $f(\alpha)$ becomes an exceedingly singular object, and check on the numerical accuracy attainable in each case. Since the singular behavior of $f(\alpha)$ is concomitant to the importance of eigenfunctions of the overlap kernel with very small eigenvalues, we are to expect larger numerical errors when $f(\alpha)$ becomes singular.

Gaussian overlap functions, being invariant under translations in the generator coordinate space, can be diagonalized by Fourier transforms [7,8]:

$$\frac{1}{2\pi}\iint e^{-i\lambda\alpha}\, e^{-\frac{(\alpha-\alpha')^2}{a^2}}\, e^{i\lambda'\alpha'}\, d\alpha\, d\alpha' = \Lambda(\lambda)\,\delta(\lambda-\lambda')$$

with

$$\Lambda(\lambda) = a\,\pi^{\frac{1}{2}}\, e^{-\frac{\lambda^2 a^2}{4}}$$

The collective hamiltonian associated with the quadratic approximation to the energy kernel reads

$$N^{-\frac{1}{2}} K N^{-\frac{1}{2}} = \frac{1}{2\pi}\int d\alpha \left[\int d\alpha' \frac{e^{-i\lambda\alpha}}{\Lambda^{1/2}(\lambda)}\, e^{-\frac{(\alpha-\alpha')^2}{a^2}} \left[E_0 + \frac{A}{2}(\alpha-\alpha')^2 + \frac{B}{2}\left(\frac{\alpha+\alpha'}{2}\right)^2\right] \frac{e^{i\lambda'\alpha'}}{\Lambda^{1/2}(\lambda')}\right]^2 \quad (3)$$

This gives just the momentum space version of a harmonic oscillator hamiltonian. The exact normalized solutions for the collective amplitudes g are thus standard harmonic oscillator wavefunctions:

$$g_n(\lambda) = \mathcal{N}_n \, e^{-\frac{b^2\lambda^2}{2}} \, H_n(b\lambda) \tag{4}$$

The corresponding weight functions are given formally as

$$f_n(\alpha) = \int \frac{d\lambda}{(2\pi)^{1/2}} \, \frac{e^{i\lambda\alpha}}{\Lambda^{1/2}(\lambda)} \, g_n(\lambda) \tag{5}$$

They are well-behaved functions only for $2b^2 > a^2$, i.e., for overlaps which are narrow in terms of the oscillator parameter b.

We study therefore the behavior of the numerical treatment of this problem via eq.(2) and compare results with the exact solution (4) for various values of the parameter

$$\gamma = \frac{a}{2b} \tag{6}$$

which determines the existence of $f_n(\alpha)$, eq.(5). The results of this comparison are sumarized in figs.1 and 2. One notices that the stable numerical solution for the ground-state and for the first excited state energies coincide with the exact values when $\gamma < 1$. In this region the weight functions are well behaved, and degrees of freedom associated with small eigenvalues of the overlap kernel are of little importance. When $\gamma > 1$, however, the solutions stabilize at values that become more and more deviant from the exact ones as γ increases, thereby also increasing the dynamical involvement

of degrees of freedom associated with small eigenvalues of the overlap kernel.

The parameter γ, which characterizes the behavior of the weight function $f_n(\alpha)$, thus characterizes also the precision that can be obtained in the numerical solution of the dicretized version of the GHW problem, for a given numerical noise. The discussion suggests moreover the general qualitative conclusion that the residual error of the numerical method for a given precision will be larger when the overlap kernel is "wide", in the sense that typical distances for the collective problem, in terms of the collective coordinate, are small compared with the characteristic width of the overlap kernel.

An alternate description of this situation can be given as follows [6,7]. The collective subspace associated with the given continuous family of generator states $|\alpha>$ is in general infinite dimensional.. Furthermore, in many cases zero is a limit point for the eigenvalues of the overlap kernel[6]. This is true, in particular, for Gaussian overlaps[7]. Under these circunstances, the eigenvectors of the overlap kernel with eigenvalue smaller than ε span a subspace of the collective space which is also infinite dimensional. The numerical solution actually ignores this subspace, ε being of the order of the unavoidable numerical noise, the numerical solution being essentially the exact solution in the remaining finite dimensional subspace. A parameter such as γ above characterizes the dynamical relevance of the ignored dimensions of the collective space, the error associated with the finite value of ε being the corresponding truncation error. This type of error can be controlled by a) treating the overlap

kernel analitically whenever feasible or b) modifying the adopted generator coordinate scheme so as to make the relevant degrees of freedom more readily accessible to numerical treatment. The latter option includes, in the present case, the use of complex generator coordinater [9,10].

We thank E.J.V. de Passos for a critical reading of the manuscript.

REFERENCES

1. D.L.Hill and J.A.Wheeler, Phys.Rev. 1953, 89 :112.

2. J.J.Griffin and J.A.Wheeler, Phys.Rev. 1957, 108 : 311.

3. H.Flocard and D.Vautherin, Nucl.Phys. 1976, A264 : 197.

4. K.Goeke, M.V.Mihailovic, K.Allaart and A.Faessler, Nucl. Phys. 1975, A243 : 440; H.Muther, K.Goeke, K.Allaart and A.Faessler, Phys.Rev. 1977, C15 : 1467.

5. L.F.Canto, Nucl.Phys. 1977, A279 : 97.

6. A.F.R. de Toledo Piza, E.J.V. de Passos, D.Galetti, M.C. Nemes and M.M. Watanabe - Phys.Rev. 1977, C15 : 1477.

7. A.F.R.de Toledo Piza and E.J.V. de Passos, Preprint IFUSP P-120, June 1977.

8. B.Giraud, J.C.Hocqueghem and A.Lumbroso; Phys.Rev. 1973, C7 : 2274.

9. D.M.Brink and A.Weiguny; Nucl.Phys. 1568, A120 : 59.

10. E.J.Veloso de Passos and A.F.R. de Toledo Piza, Collective Dynamics, Generator Coordinates and Weyl Systems, submitted to the 1977 Meeting of Sociedade Brasileira para o Progresso da Ciência. Ciência e Cultura.

FIGURE CAPTIONS

Figure 1 Numerical errors for some truncation levels in (a) the ground state energy, and (b) transition energy. Each curve is labeled by the parameter γ associated with it. Solid lines serve only to guide the eyes.

η is defined as $\eta = -\ln(\epsilon)/\ln(10)$

Figure 2 Rate of change of the numerical errors in the ground state energy for the same set of γ's. Solid lines serve only to guide the eyes.

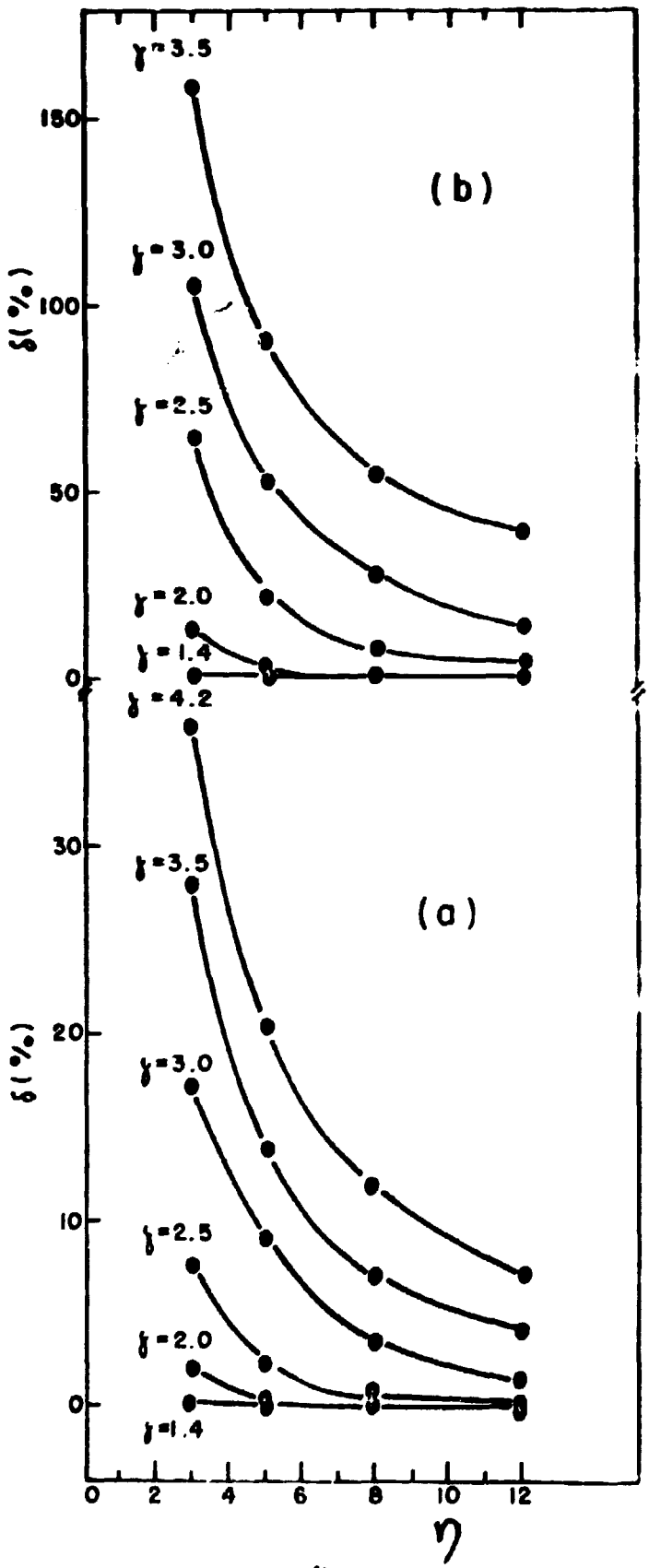

γ=3.5
150
(b)
γ=3.0
δ(%)
100
γ=2.5
50
γ=2.0
γ=1.4
0
γ=4.2
30
γ=3.5
(a)
20
γ=3.0
δ(%)
10
γ=2.5
γ=2.0
0
γ=1.4
0
2
4
6
8
10
12
η

fig. 1

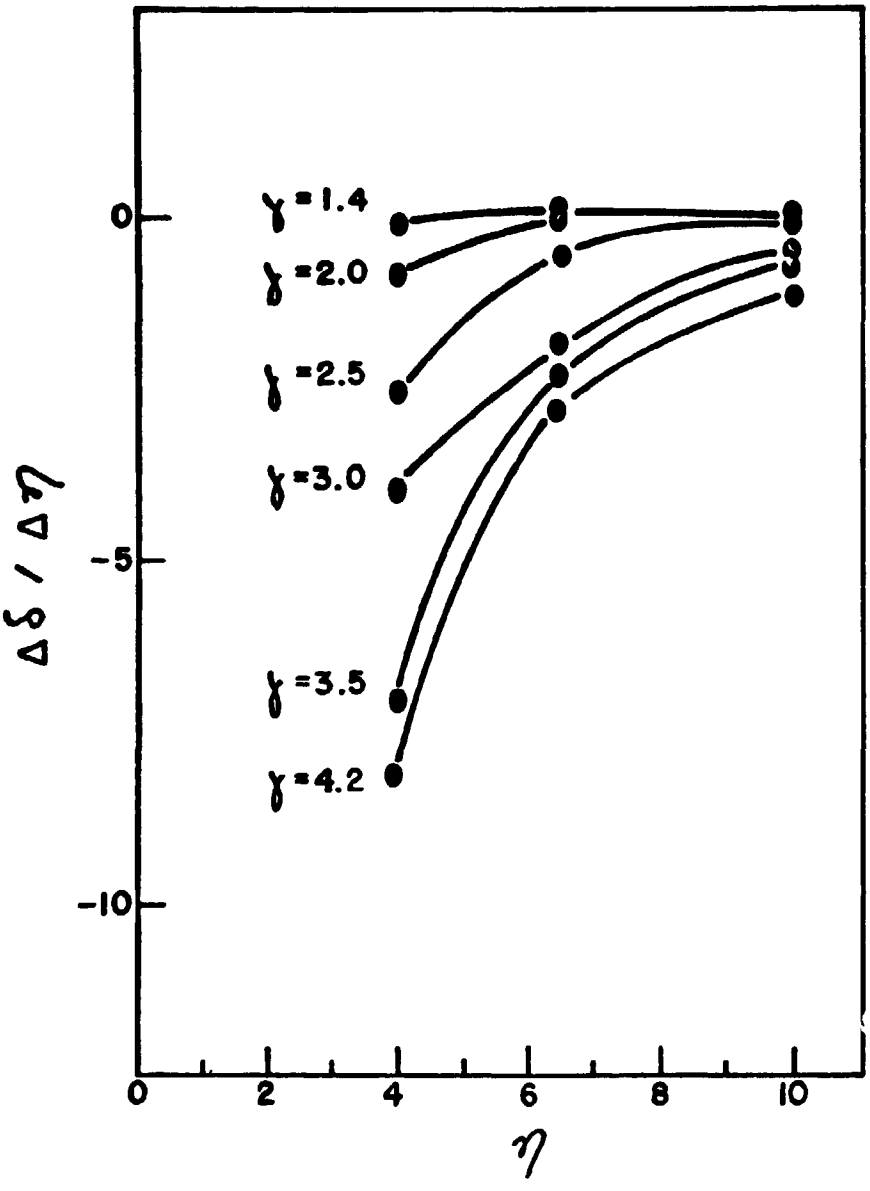


fig 2